Five-Zone Simulating Moving Bed for Ternary Separation

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ABSTRACT: *Five-zone Simulating Moving Bed (SMB) system, designed for ternary separation, is a modified form of standard four-zone SMB which is only effective in binary separation. It was reported in literature that the five-zone SMB separates the extract-II stream with a lower purity value than that of raffinate and extract-I streams. To address this issue, five zone SMB was designed, using safety margin method for the separation of a ternary amino acid mixture comprises of methionine, phenylalanine and tryptophan having linear isotherms values. The operating conditions at fixed zone-I flow rate were calculated by using triangle theory and the developed mathematical model was run for the simulation studies with Aspen Chromatography vis 12.1. (2004) simulator. The simulation results of the 2-extract five-zone SMB system were illustrated for the effect of change in zone safety factor (β_2, β_3 and β_4) values on the separation performance (product purity and recovery) and on solutes band propagation behavior at cyclic steady state.*

KEY WORDS: *Five-Zone SMB, Zone safety factor, Simulation, Separation, Wave dynamics.*

INTRODUCTION

The continuous Simulating Moving Bed (SMB) is among one of the rising interests in the field of bioseparations and biotechnology because of its diverse advantages such as reduction of solvent consumption, operates on continuous large scale operation, better exploitation of the adsorbent [1,2] low investment cost, high productivity, purity and yield, less manpower and operational floor space [3,4]. Simulating moving bed process has found numerous applications in the field of purification or separation of chiral drugs, biochemical products, optical isomers, organic solvents, sugars and fractionation of isotopes [1,5-8].

In bioproduct purification process, it is often demanded to have ternary separation, two or multiple SMB units should be connected in series and operated simultaneously [2,8]. However, such arrangement leads to process complexity and have much higher operating and maintenance costs, compared to the use of single SMB unit [2]. Certainly, it is economical to separate ternary mixtures with desired purity and recovery values in a single SMB unit.

As reported elsewhere [9-12], several researchers, *Wooley et al.* (a nine zone SMB), *Wankat* (easy split multiple SMB units), *Silva & Rodrigues* (JO SMB system), have made tremendous contributions in designing of SMB process for the separation of quaternary and ternary mixtures. While several research teams, *Navarro et al., Beste & Arlt, Kim et al., Wang & Ching,*

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Abunasser & Wankat, Jo et al., Mun, Khan and Younas [2,8,13-19], have focused in their research work on the design, optimization, modeling and influence of bed subdivision on wave dynamics and separation performance, efficient control of operation strategies and the effect of zone flow rate with the constraint of fixed feed flow rate on a single SMB unit with five-zone [2,8,13-15,17-19]. Despite the fact that, extensive research studies can be found in literature relating five-zone SMB operation, but still it was known to have limited operations for ternary separation due to unresolved problems. The unresolved limitation of the extraction of extract-II stream with a lower purity value than that of raffinate and extract-I streams needs attention, because such an inevitable limitation restricts the application scope of five-zone SMB in ternary mixture separations.

The aim of this study is to determine favorable operating conditions, at the constraint of fixed zone-I flow rate for overcoming the aforementioned disadvantage in the current five-zone SMB process for ternary separation. For this objective, the SMB system was modeled, using safety margin method [20] and operating conditions were calculated by using the triangle theory [21]. The process improvement for higher product purity and recovery values in relation to the solutes band migration behavior at cyclic steady state under the influence of change in separation zone safety (zone flow rate βj, j = 2, 3, 4) factor values were investigated by conducting detailed simulating studies with Aspen Chromatography vis 12.1. (2004) simulator, taking into accounts both the axial dispersion and mass transfer effects.

SMB MODEL FORMULATION

The mathematical model for five-zone simulating moving bed system was developed based on the following assumptions.

- No concentration gradient within the film of the particle (lumped film mass transfer model, because it has sufficient advantages in the aspect of simplicity with linear system, accuracy and computation time).
- No chemical reaction.
- No phase change other than adsorption.

For the SMB model, the single porosity model [22] was adapted for component i within each zone for the mobile phase as follows:

$$\frac{\partial C_i}{\partial t} + PK_{f,i}(C_i - C_i^*) = -u_o^j \frac{\partial C_i}{\partial Z} + E_{b,i}^j \frac{\partial^2 C_i}{\partial Z^2} \quad (1)$$

Where C_i is the mobile phase concentration of component i at time t and axial position z; j is the zone number (I, II, III, IV, V) and u^j_o is the mobile phase interstitial velocity in zone j; and P is the phase ratio defined as:

$$P = \frac{1-\varepsilon}{\varepsilon} \quad (2)$$

Where ε is the total void fraction; $E^j_{b,i}$ is the axial dispersion coefficient of the component i in the zone j and is defined from *Chung & We*n correlation (23):

$$\frac{E_{b,i}^j}{vd_p} = \frac{\varepsilon}{0.2 + 0.0011R_{ep}^{0.48}} \quad (3)$$

Component mass balance in the pore phase is given by the following Eq. (24):

$$(1-\varepsilon_P)\frac{\partial C_i}{\partial t} + \varepsilon_p \frac{\partial C_i^*}{\partial t} = K_{f,i}(C_i - C_i^*) \quad (4)$$

$$K_{f,i} = a_p k_m \quad (5)$$

Whereas C_i^* is the average pore phase concentration, C_i is the adsorbed phase (solid-phase) concentration and ε_p is the intra-particle void fraction. $K_{f,i}$ is the lumped mass transfer parameter which includes the effects of both film mass transfer and intra particle diffusivity; k_m is the overall mass transfer coefficient and is used as input parameter for the Aspen simulation with the linear isotherm; a_p is the external surface area per unit particle volume. For spherical particle a_p = 3/R, where R is the solid particle radius. The Initial Conditions (I.C) and Boundary Conditions (B.C) for each column are:

$$t = 0, \quad C_i(t,z) = 0 \text{ and } C_i^*(t,z) = 0 \quad (6)$$

$$z = 0, \quad \frac{\partial C_i}{\partial z}\Big|z=0 = \frac{u_o}{E_{b,i}^j}\left[C_i(t,z=0) - C_{i,in}(t,z=0)\right] \quad (7)$$

$$z = L_c, \quad \frac{\partial C_i}{\partial z}\Big|z=0 = 0 \quad (8)$$

Where the inlet concentration of the component i is designated by $C_{i,in}$.

For our proposed amino acid mixture system i.e., methionine, phenylalanine and tryptophan having linear

Table 1: System parameters for 2-extract five-zone SMB simulation [25].

Length of the column (cm)	25		
Dia of the column (cm)	2.5		
Particle radius (cm)	0.0181		
Mobile phase density (g/cm^3)	996		
Liquid viscosity (cP)	0.89		
Inter-particle voidage (ε_i)	0.346		
Intra-particle voidage (ε_p)	0.55		
	Methionine	Phenylalanine	Tryptophan
Feed concentration (g/L)	0.5	0.5	0.5
Axial dispersion coefficient (cm^2/min)	The *Chung & Wen* correlation (1968)		
Mass transfer coefficient (1/min)	0.0518	0.0171	0.0157
Linear isotherm parameters	0.3537	1.6015	11.771
Adsorbent: Poly-4 Vinyl pyridine (PVP) resin			

isotherm values, the equilibrium relationship between C_i and C_i^* is usually expressed by a linear adsorption isotherm model given as follow:

$$C_i = K_i C_i^* \quad (9)$$

where K_i is the linear-isotherm parameter.

Characteristic parameters of the model system

The feed concentration of each of the amino acids was set equal to 0.5 g/L. The intrinsic parameters and linear isotherm values were the same as that of *Lee*'s [25] work. All the simulation parameters necessary for modeling of the current five-zone SMB system are summarized in Table 1. Aspen Chromatography vis 12.2 (2004), simulator was used for the numerical computation, which has been validated in several studies found in literature [8, 10, 15-19]. To solve the model equations for the product recovery and purities, a Biased Upwind Differencing Scheme (BUDS) was employed with implicit Euler integration having a step size of 0.05.

Design of operating conditions

One of the key issues in SMB process is designing and its successful operation, which depends on the correct choice of operating conditions, such as determination of each zone flow rate and column switching time. Due to the complex behavior of these units the choice of fixing the operating conditions is not straightforward, currently used SMB design approaches are safety margin method [20], standing wave design method [24,27], triangle theory [21,28], separation volume [29-31] and the method based on consideration of velocity of propagation of specie concentration [32].

The operating conditions for the linear ternary separation system of the current work were calculated by using the triangle theory [21], an important SMB design methodology, it allows one's to find a feasible zone where separation is obtained for both linear and non-linear isotherm systems. Although equilibrium models are powerful design tools, the conditions may not entirely be applied in the design of real SMB units, because mass transfer and axial dispersion effects are often present [29]. Therefore, the correct adjustment of the internal flow rates is the key parameter in the design of SMB process, the flow rates are regulated in a way that the simultaneous functioning of all the zones are guaranteed. Hence, these effects have been taken into account by using a safety margin factor (β) in the equilibrium models, whose value is endorsed randomly and may lead to over-or underestimating errors [29]. In this regard, safety margin method was effectively used for the design of SMB with mass transfer resistance [2,8, 33-35].

To calculate the explicit operating conditions the corresponding zone-I flow rate was kept constant. Moreover, equimolar feed compositions were assumed and for the determination of other flow rates the

equilibrium theory in combination with a safety factor (β) value was used. Furthermore, the advantage of this approach is that the flow rate ratio is a dimensional group bringing together information about the column volume, V, unit flow rates Q_j, and switch time, t^*, thus can be applied whatever is the configuration and size of the SMB unit in both linear and non-linear systems.

For the desired separation of the ternary amino acid mixture a single cascade 2-extract five-zone SMB as shown in Fig.1 was applied to separate the mixture into three different fraction. The solute C (tryptophan) in extract-I stream, solute B (phenylalanine) in extract-II stream and the solute A (methionine) in the raffinate stream respectively. The SMB system was designed with the safety margin method, this method is based on the following relationship between the migration velocity of the key solute in each zone and the average port velocity.

$$u_C^I = \frac{u_0^I}{1+\left(\frac{1-\varepsilon}{\varepsilon}\right)K_C} > v \qquad (10a)$$

$$u_B^{II} = \frac{u_0^{II}}{1+\left(\frac{1-\varepsilon}{\varepsilon}\right)K_B} > v \qquad (10b)$$

$$u_A^{III} = \frac{u_0^{II}}{1+\left(\frac{1-\varepsilon}{\varepsilon}\right)K_A} > v \qquad (10c)$$

$$u_B^{IV} = \frac{u_0^{IV}}{1+\left(\frac{1-\varepsilon}{\varepsilon}\right)K_B} < v \qquad (10d)$$

$$u_A^V = \frac{u_0^V}{1+\left(\frac{1-\varepsilon}{\varepsilon}\right)K_A} < v \qquad (10e)$$

Where u^j_i is the migration velocity of the component i (A, B and C) in zone j (I, II, III, IV and V), v is the port moment velocity (single column length/switching time), u_o is the mobile phase interstitial velocity in any zone and K_i is linear isotherm parameters of component i. The Eqs. 10(a) to 10(e), describe all the feasible zone linear velocities and the port movement velocities that guarantee the separation of the desired components in the separation zones of the 2-extract five-zone SMB system. For successful operation of the system, the aforementioned

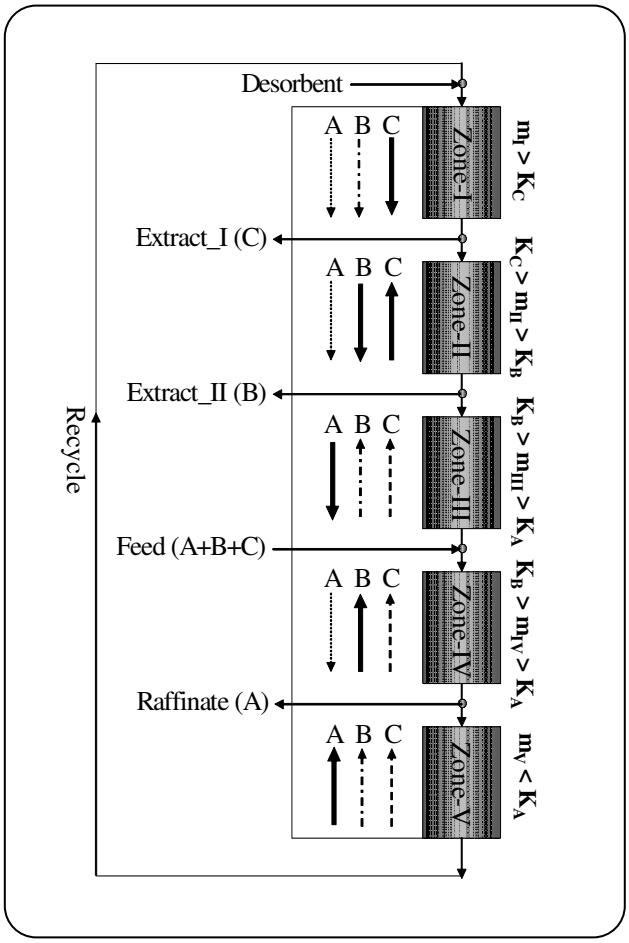

Fig. 1: 2-extract five-zone SMB for ternary separation, where the ideal direction of solute migration (relative to the ports) for successful ternary separation is indicated by bold heavy arrows. A: Lowest-affinity solute; B: Intermediate-affinity solute; C: High-affinity solute.

equations must be satisfied with or without mass transfer resistance. To obtain high purities values of the extract-I, extract-II and raffinate product streams, the operating points are required to be in the complete separation region. Theoretically, the complete separation region can be determined by flow constraint in the zones of the 2-extarct five-zone SMB system. The conditions for complete separation among the components can be easily expressed in term of net flow rate ratio of each zone of the unit. To achieve complete separation of the ternary components the net flow rate of the lowest-affinity solute (A, methionine) must be conveyed to raffinate outlet stream, intermediate-affinity solute (B, phenylalanine) must be passed to extract-II outlet stream and highest-affinity solute (C, tryptophan) must be conveyed to

the extract-I outlet stream respectively. For these considerations, the aforementioned five constraints can be re-expressed into zone flow rate ratios (m_j), linear isotherm parameters (K_i) and safety factor (β) based on the safety margin method as fallows:

$$m_1 = \beta K_C \quad (11a)$$

$$m_2 = \beta K_B \quad (11b)$$

$$m_3 = \beta K_A \quad (11c)$$

$$m_4 = K_B / \beta \quad (11d)$$

$$m_5 = K_A / \beta \quad (11e)$$

The parameter m_j, so called flow rate ratio, defined as ratio of the net fluid flow rate over the solid phase flow rate in each zone of the SMB unit [21].

$$m_j = \frac{\text{net fluid flow} - \text{rate}}{\text{adsorbed phase} - \text{rate}} = \frac{Q_j^{SMB} t^* - V\varepsilon^*}{V(1-\varepsilon^*)} \quad (12)$$

Where Q_j^{SMB} is the internal flow rate in each zone of the 2-extract SMB, ε^* is the overall void fraction, t^* is the column switching time and V is volume of the column. The zone flow rate ratio, m_j can further be related to the interstitial velocity and port movement velocity as given by [28].

$$m_j = \frac{u_0^j - v}{(\frac{1-\varepsilon}{\varepsilon})v} = \frac{u_0^j t^* - L_C}{(\frac{1-\varepsilon}{\varepsilon})L_C} \quad (13)$$

L_C is the single column length.

To maintain desired product purities against mass transfer resistance, the value of β in the above equations, usually chosen to be greater than unity. To have simple SMB process operation, approach like same β value for each zone may be used [8]. However this approach may have some possibility of loosing the global optimum. Because once β is selected, all the flow rates (extract-I, extract-II, raffinate and desorbent flow rates in each section) are fixed with respect to feed flow rate. Successful operation of SMB unit with same β value approach has been employed in several researcher's studies [2,8,33-36]. In this study, a new methodology has been adopted, the flexibility of varying the safety factor, β_j, (j = 2, 3, 4) value under the constraint of fixed zone-I flow rate in any one of these separating zone, in comparison to the existing and preferred one, i.e. same β value for each zone. Because, of having the goal that, the influence of different β_j values on the separation performance is one of the important issue in five-zone SMB research.

RESULTS AND DISCUSSION

The detailed simulations studies were carried out for the 2-extract five-zone SMB with one column per each zone by varying the magnitude of the safety factor (β) value under fixed zone-I flow rate i.e., 30 L/min.

The simulation results in terms of product purity values were plotted as a function of safety factor (β) value as shown in Fig. 2, while the corresponding operating points for the product purities values were plotted in the rectangular diagram (m_3 Vs m_2) and triangular diagram (m_3 Vs m_4) as presented in Fig. 3 to make sure that these points were within the valid operating area. Keeping zone-I flow rate constant, it was observed that the purity value of raffinate product stream and extract-I product stream increases with increase in safety factor (β) value. The purity value of solute B in the extract-II product stream also rises with increase in β value. But such enhancement in purity of B is up to a value of β after that further increase in the β value causes the purity value to decrease.

Keeping zone-I flow rate constant, increase in the value of β results in a decrease of feed flow rate to the system. In addition, an increase in switching time as well as increase in the difference of feed flow rate ratios, m_2 and m_3 also resulted. As a consequence, enhancement in the purity values of both raffinate stream and extract-I stream occurs.

As expected from equation, $m_4 = K_B/\beta$, an increase in β value decreases the zone-IV flow rate, which may affect the solute velocities of component B. The adsorption wave of solute B in zone-IV migrates slower (thus becomes further away from the raffinate port) and may results to enhance the purity of solute A. Other factor which may cause the purity of solute A to increase is the high value of zone-I flow rate as compared to other zones flow rates though increase in β value has no effect on zone-I flow rate, because it wass kept fixed i.e., 30 L/min. At this value may be the solute wave velocity of C migrates easily in zone-I (that can enhance the efficiency by regenerating the column in zone-I) and helps to improve the product purity of raffinate stream.

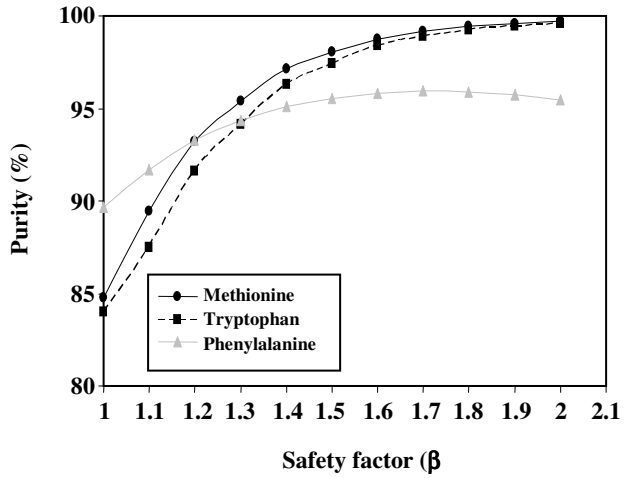

Fig. 2: Influence of change in safety factor (β) value on the performance of the 2-extract five-zone SMB keeping zone-I flow rate constant.

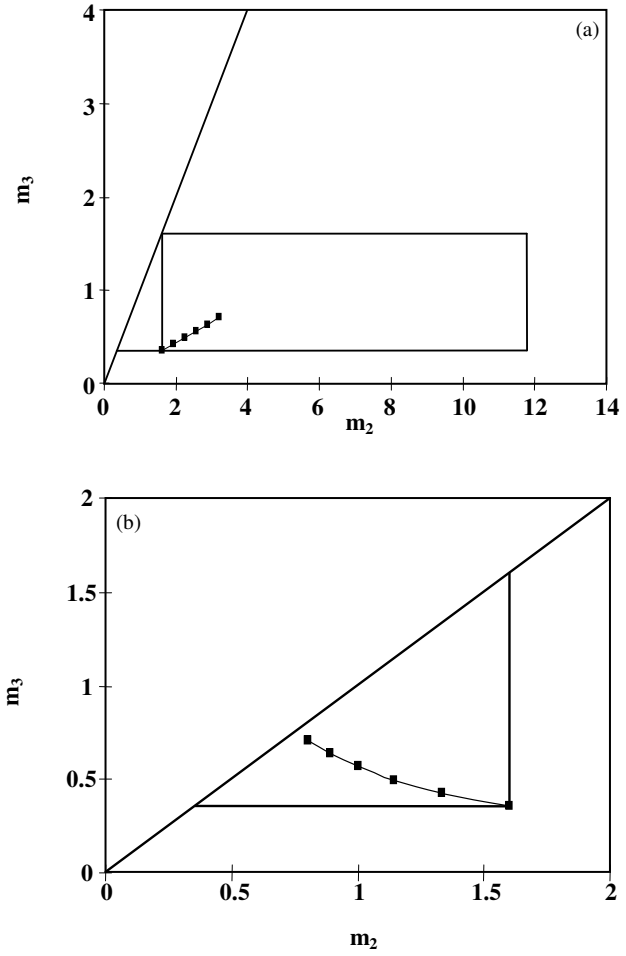

Fig. 3: Operating diagrams for 2- extract five-zone SMB [19] (a) m_3 - m_2 (around the extract-II port), (b) m_3 - m_4 (around the feed port).

Purity of extract-1 product stream has also noted to increase with increasing β value. The desorption wave of B diffuses rapidly towards the zone-II column end as according to equation, $m_2 = \beta K_B$, along with this, the flow rate of zone-V decreases with increase in β value respectively. Both these factor may results to enhance the purity of C, because the solute wave velocity of B in zone-II and that of A in zone V becomes further away from the extract-I port.

As said earlier, the purity of solute B in extract-II stream also increases with rise in β value. The improvement in purity value may be due to the reason that the adsorption wave of A in zone-III migrates faster as given by equation, $m_3 = \beta K_A$, thus solute A becomes further away from the extract-II port. This may help to prevent possible contamination of A with B in extract-II stream. Also, the solute wave velocity of C migrates slower in zone-II due to decrease in flow rate, this may also helps to improve the purity of B in extract-II product stream. However, due to fast increase in port switching time with further rise in β value, results in easy approach of solute C adsorption wave towards the column end. This may leads to possible contamination of C in extract-II product stream. Other factor that may elucidate the decrease in the purity value of B is that, as stated earlier that the port switching time increases sharply with increase in value of β specifically after 1.6. This may cause the solute wave of C to diffuse easily towards forward direction in zone-III, upon port switching the solute C reaches the extract-II port earlier that significantly contaminates B. In view of the purity results of solute B it seem that the solute wave velocity of C acts to increase the purity value of B up to β value of 1.6 beyond this value further increase in β value makes solute C to contaminates the extract-II product stream as explained earlier. Furthermore, Table 2 illustrates the desorbent and adsorbent requirement and unit productivity.

Influence of zone safety factor (zone flow rate β)

In the earlier section, the separation performance of the 2-extract five-zone SMB for the ternary mixture was illustrated in term of product purities on the restriction that same safety factor (β) value was used for each zone just for the sake of simplicity, as been successfully applied in several previous studies as stated elsewhere [2, 8, 20, 33]. In real operation it is necessary to vary the

Table 2: Definition of process parameters for 2-extract five-zone SMB.

Unit parameter definition			Value	
Desorbent requirement, DR (cm^3/min per cm^3/min-feed) = Q_D / Q_F				
β	Q_F (cm^3/min)	Q_D (cm^3/min)	Q_D / E_F	10^{-3} Pr (min^{-1})
1	0.0024	0.02418	9.14	4.3
1.2	0.0017	0.02512	15.19	2.6
1.4	0.001	0.02579	25.01	1.7
1.6	0.0006	0.02630	42.80	1
1.8	0.0003	0.02670	83.03	0.5
2	0.0001	0.02703	251.26	0.1
Adsorbent requirement, AR (cm^3) = N_{col} * V_{col}			613.6	
Productivity, Pr (cm^3/min-feed per cm^3-solid) = Q_F / Volume of solid (AR)				

zone safety factor values (β, zone flow rates) to make any SMB system work against the desired separation. Hence, to meet this objective, an approach of changing the β value among the different zones was applied. Therefore, in this section, the effect of the individual zone safety factor (zone flow rate β_2, β_3 and β_4) value on the separation performance of the five-zone SMB is investigated at fixed zone-I flow rate, an issue of significant importance for the operation and design of the five-zone SMB systems. Moreover, to further explain the separation phenomena, solutes band migration behaviors at cyclic steady state were examined at different column switching periods. Detailed simulation studies were performed for the column profile study under the effect of change in β_2, β_3 and β_4 values, and the results illustrated here are for those values of safety factors which gives maximum purity index (PI) value for the ternary system. The purity index (PI), which has often been used to indicate the separation performance of a given process [8, 16-18, 26], and is defined as the average of the purities of the three components as fallows.

$$PI = \frac{(\text{purity of A}) + (\text{purity of B}) + (\text{purity of C})}{3} \qquad (13)$$

Influence of zone safety factor (zone flow rate β_2) value in section II

To investigate the effect of safety factor, β_2 on the separation performance of five-zone SMB, its value was varied in section-II while keeping the other zone safety factor, β_j (j = 1, 3, 4, 5) values constant as illustrated in Fig. 4.

The purity trend demonstrates that increase in the value of β_2 cause no effect on the purity value of methionine. For tryptophan, the purity value rises in the extract-I stream with the increase in the value of β_2, because, the desorption wave of solute B migrates faster in zone-II as expected from Eq. 11(b). Thus becomes further away from the extract-I port and may cause the purity value of tryptophan to increase.

Phenylalanine purity in extract-II product stream decreases, although its solute wave velocity increases in zone-II as anticipated from equation, $m_2 = \beta K_B$. This may favors to enhance the diffusing wave of B towards the column end and results an increase in its purity value. However, as the value of β_2 increases, the zone-II flow rate increases as well, which may cause the solute wave of C to diffuse more towards the extract-II port and thus acts to contaminate solute B. Table 3, demonstrates the recovery values for the three product stream under the influence of change in β_2 value. A general trend of enhancement in the recovery values was observed with the rise in the safety factor, β_2 value.

A typical SMB cyclic operation always involves continuous input of feed to the system and a recycle from the last zone to the first zone (desorbent inlet port). In our described system, 2-extact SMB the recycle stream exit from zone-V and enters at zone-I having the desorbent inlet port. Once, the operation begins, the solute waves propagate and their concentration along the bed increases

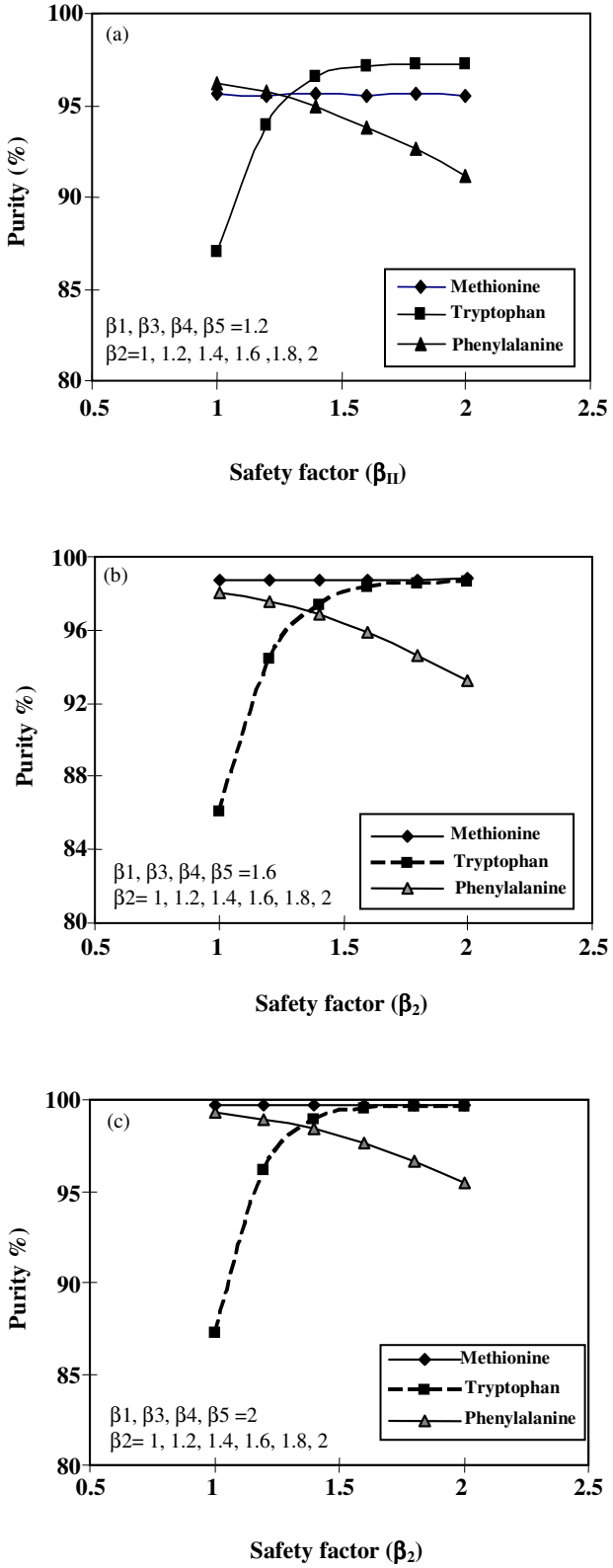

Fig. 4: Influence of change in β_2 value on the separation performance of the 2-extract five-zones SMB.

gradually, such state may be mentioned as transient period. During this transient period each solute band growth proceeds continuously until becomes fully developed. Even though at the fully developed stage the solute wave concentration varies instantaneously (see Fig. 5) at any position relative to the feed port making it impossible to have a constant form (static steady state) of solute band with respect to time and position. However, if one's observed a series of solute wave migration behavior, comes to know that the solute band exhibits a uniform repeating pattern at every switching time. Such state, where the migration of the solute waves shows a cyclic behavior in every switching period has been defined as "cyclic steady state" [17, 25].

Fig. 5 shows the cyclic steady state profile of the solute bands migrating along the different sections of five-zone SMB under the influence of change in β_2 value only. These solute bands are always accompanied by two concentration waves, defined as absorption and desorption waves. It is the ranges of these two waves, which determine the product purities of the components system [17]. Evaluating Fig. 5, the feed mixture enters through the feed port, the adsorption wave of solute A (fast moving component) migrates downward in zone-IV and its concentration increases continuously at the raffinate port as shown in the Fig.5(a). In zone-V the solute wave of A gradually moves towards the column end as depicted in Fig.5(b,c), which may cause slight contamination of extract-I product stream, but at the mean time due to port switching such phenomena may results to increase the concentration of raffinate product stream and thus restrict the possible contamination. As a result the adsorption and desorption wave of solute A is well confined within zone-III, IV (where the solute wave velocity of A is higher than the v_{port}) and zone-V (solute velocity of component-A is lower than the v_{port}) respectively. If the adsorption wave of A is not confined with the described zones, the extract stream may be contaminated with solute A. Simultaneously, The adsorption and desorption wave of solute B are well confined in zone-II and IV respectively. In zone-II the solute wave velocity of B is higher than the v_{port}, such constraint may results in higher concentration of B in the extract-II stream. As illustrated in Fig. 5(a,b) the adsorption wave of B is migrating rapidly in zone-II towards the extract-II product port and become fully developed (see Fig. 5c),

Table 3: Effect of change in β_2 value on the separation performance (recovery) of the 2-extract five-zone SMB.

	Product recovery (%)		
	Raffinate Methionine	Ext_1 Tryptophan	Ext_2 Phenylalanine
$\beta_1, \beta_3, \beta_4, \beta_5 = 1.2$	93.56	95.93	80.50
	93.49	94.84	89.53
	93.22	92.07	91.23
	93.34	93.57	92.61
	93.12	90.34	94.60
	93.02	88.40	94.44
$\beta_1, \beta_3, \beta_4, \beta_5 = 1.6$	97.98	98.74	84.22
	97.87	98.17	89.32
	97.79	97.40	97.63
	97.72	96.41	98.74
	97.66	95.17	98.86
	97.60	93.69	98.99
$\beta_1, \beta_3, \beta_4, \beta_5 = 2$	99.54	99.37	85.01
	99.51	98.98	95.98
	99.48	98.15	98.96
	97.46	97.64	99.53
	99.43	96.62	99.61
	99.41	95.35	99.58

such wave migration may prevent its possible contamination with other feed components. Solute C (tryptophan), which plays a major role in complete separation in five-zone SMB, exhibits a quite different pattern of solute wave migration than those of solutes A and B. The solute C wave is in the form of tooth-shape, expanding in three different zones. Due to high affinity of C (high K_C value), the adsorption wave is developed in zone-IV, where the solute wave velocity is lower than v_{port}, this may makes solute C to lag behind from the other solute waves in zone-IV. Each time the port switches, the column containing the adsorption wave of C is shifted more towards column end, such diffusion may be due to axial dispersion and mass transfer (17) effects (see Fig. 5c), as a consequence this may slightly effect the purity of B, but such effect is quite unimportant as the purity value of B is well higher than 98%. Moreover, the effect of solute C on the purity of A at the raffinate port is also insignificant, as predicted from Fig.5(a,b,c) the desorption wave of C is well confined in zone-IV, thereby preventing its possible contamination with solute A (purity 99%) in the raffinate stream.

Influence of zone safety factor (zone flow rate β_3) value in section III

Fig. 6 demonstrates the effect of change in the zone safety factor β_3 value on the product purity values keeping all the other zone safety factor values, β_j (j = 1, 2, 4, 5) constant.

The purity trends of methionine and tryptophan shows no effect with increase in the value of β_3. However, the purity trend of phenylalanine shows a steep increase with rise in the value of β_3. This enhancement in the purity value of B happens, because of the faster migration of solute A from the zone-II column end due to its increase in the solute wave velocity as predicted by Eq. 11(c). This may results to prevent solute A possible contamination with solute B and as a consequence enhance its purity in the extract-II stream. Table 4,

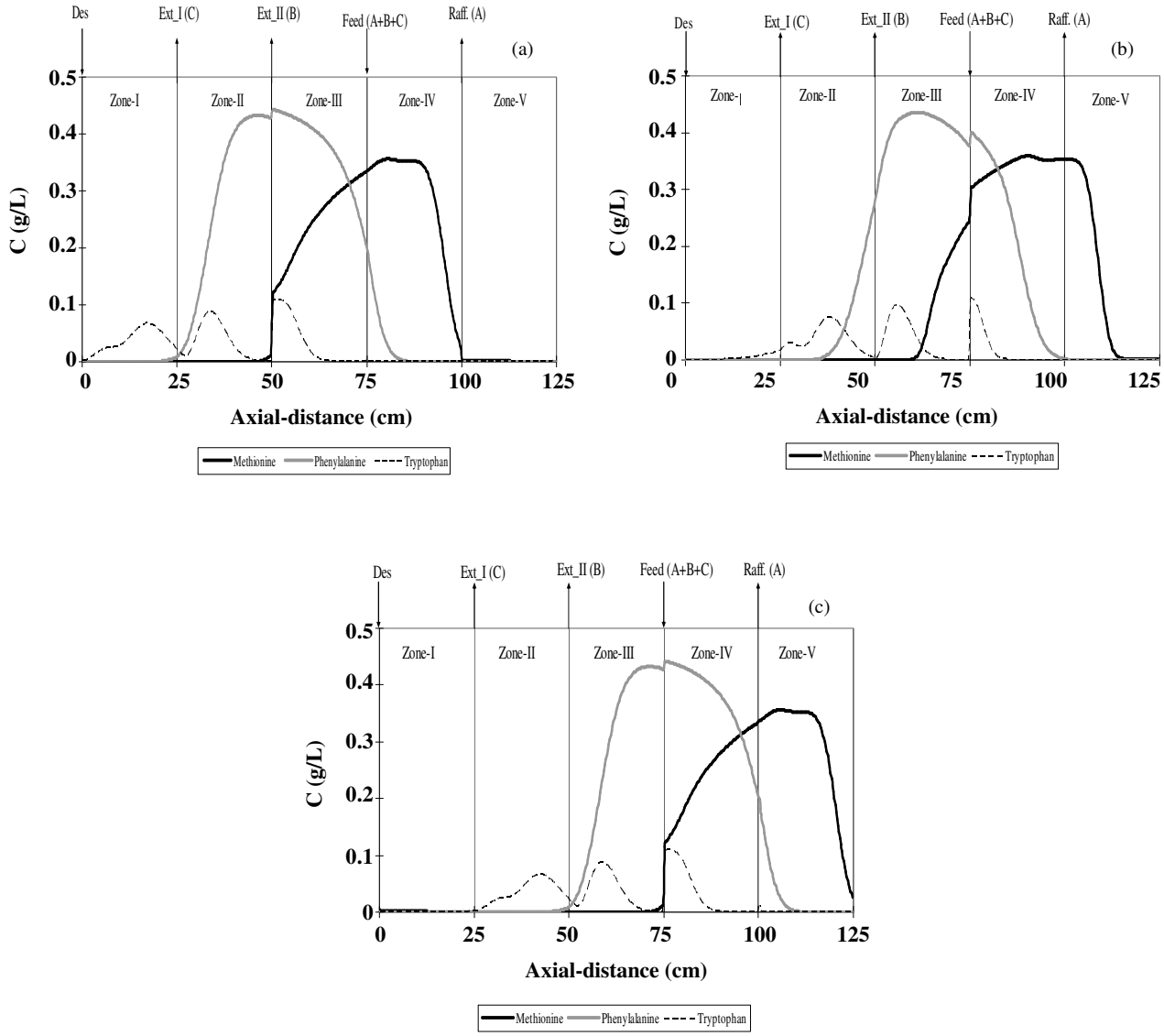

Fig. 5: Solute band migration behavior at cyclic steady state during the entire switching period in a five-zone SMB (a)At the beginning of the period (b) at the middle of the period (c) at the end of the period,. β_2 = 1.4, β_1, β_3, β_4, β_5 =2, Purity (Methionine =99.74%, Tryptophan = 98.92% and Phenylalanine = 98.38%), P.I value = 99.02%.

illustrates the product recovery values under the influence of change in β_3 only, maximum recovery values were reported for highest value of β_3 i.e. 2 while fixing other safety factor values , β_1, β_2, β_4, β_5 at the value of 2 also. At such zone safety factor values, column switching time is maximum, in addition the flow rate at zone-1, zone-II, zone-IV decreases. All this favors the respective solute bands to reach the designated exit column ends and recovered fully before switching of columns happens.

Fig. 7 demonstrates the cyclic steady state of the solute bands under the influence of change in the value of β_3 only. Similar behavior of adsorption waves of both solute A and B is absorbed in comparison to that of only change in β_2 value (see Fig. 5). But a slightly faster migration behavior was observed in zone-II for the desorption wave of solute B as shown in Fig. 7(a,b), as a result of increase in zone-II flow rate and becomes fully developed by the end of the switching time as depicted in Fig. 7(c), as a consequence, the purity value of tryptophan increases. However, for solute C, the adsorption wave is dispersed towards zone-II column end as demonstrated in Fig. 7(a,b,c), which may due to longer

Table 4: Effect of change in β_3 value on the separation performance (recovery) of the 2-extract five-zone SMB.

	Product recovery (%)		
	Raffinate Methionine	Ext_1 Tryptophan	Ext_2 Phenylalanine
$\beta_1, \beta_2, \beta_4, \beta_5 = 1.2$	91.39	94.78	89.75
	93.49	94.84	88.99
	94.70	94.90	89.29
	95.64	94.96	88.44
	95.73	95.03	88.73
	95.94	95.11	87.77
$\beta_1, \beta_2, \beta_4, \beta_5 = 1.6$	92.19	96.53	98.61
	95.22	96.48	98.74
	96.87	96.44	98.61
	97.72	96.41	98.73
	98.15	96.37	98.60
	98.38	96.35	98.73
$\beta_1, \beta_2, \beta_4, \beta_5 = 2$	91.45	95.84	99.64
	95.56	95.74	99.64
	97.65	95.64	99.61
	99.75	99.62	99.62
	99.74	99.62	99.61
	99.72	99.61	99.58

column switching period as well by mass transfer and axial dispersion effects [30, 37,38]. In effect may contaminate solute B by decreasing its purity to 95.47% in the extract-II product stream.

Influence of zone safety factor (zone flow rate β_4) value in section IV

The results presented in Fig. 8, illustrate that only an increase in the zone safety factor (zone flow rate, β_4) value of section IV, favors the improvement in the purity value of methionine. The reason may be the adsorption wave of solute B diffuses slowly towards the raffinate port due to increase in β_4 value as expected from Eq. 11(d). Furthermore, the flow rate of zone-IV is decreasing as zone-I flow rate is kept constant, which may further decrease the solute wave velocity of B and C in zone-IV. Both these factors may results to enhance the purity value for solute A in the raffinate stream. The purity trends for the rest of the two components i.e. solute B and C, demonstrates that the purity value decreases with increase in β_4 value up to 1.4 and 1.6 respectively, after that both the solute purity values start to improve, because of high port switching time with further rise in β_4 value. Table 5, illustrates the products recovery values under the influence of change in β_4 value. The recovery values of extract-II stream product were rising with increase in β_4 value in comparison to extract-I stream product recovery. This happens as a result of decrease in zone-II flow rate (favors to decrease the phenylalanine wave diffusion to other zones), while increase in desorbent flow rate with rise in β_4 value causes the flow rate in zone-I to increase (see flow sequence in Fig. 2), in combination zone-I will have the highest flow rate, which may cause fast diffusion of the solute A wave, which may enters to zone-I, all this lowers the recovery of tryptophan.

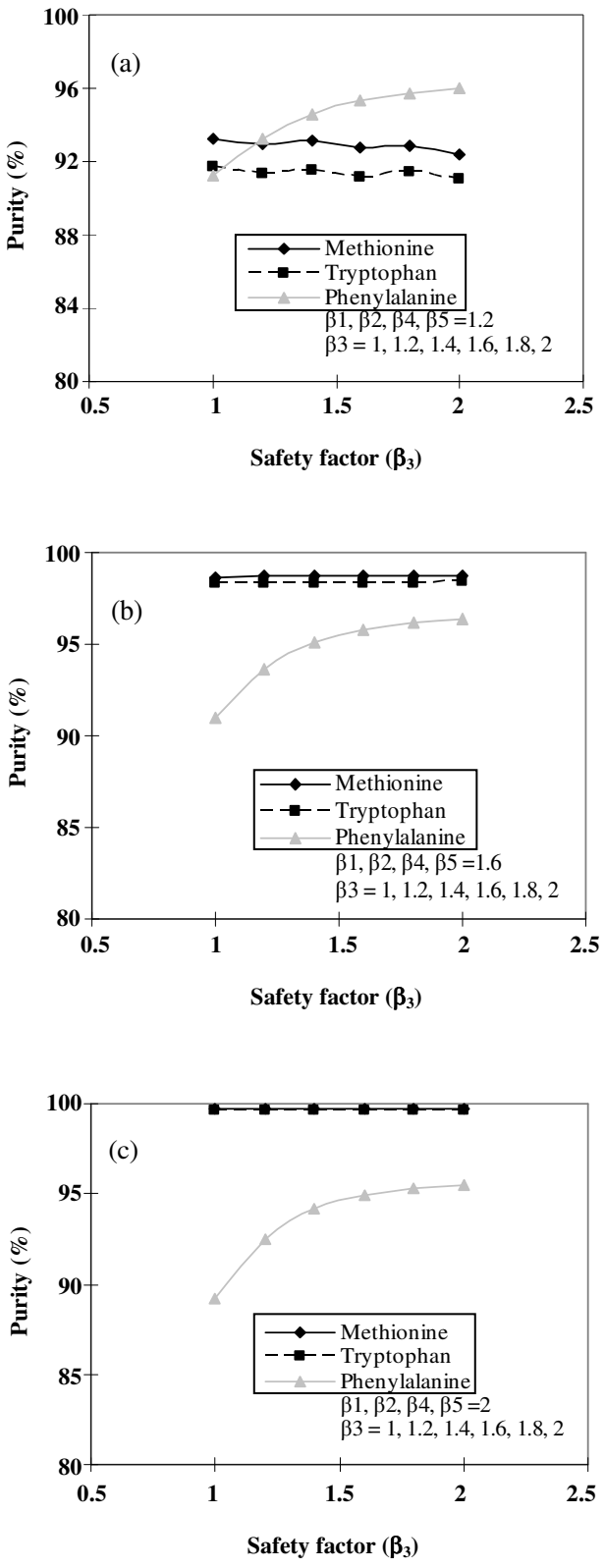

Fig. 6: Influence of Change in β_3 value on the separation performance of the 2-extract five-zone SMB.

Fig. 9 demonstrates that the desorption wave of solute B is diffused more towards to extract-II column end as a result of increase in switching time, although the flow rate in zone-II decreases (which may restrict the diffusion of solute C towards extract-II column end) with only increase in the value of β_4, as a consequence the purity of phenylalanine increases. In comparison to the solute B wave concentration as predicted in Figs. 5 & 7, the solute B concentration band examined with only change in β_4 value are shorter and this may be due to the increase in extract-II drawoff flow rates.

CONCLUSIONS

Separation performance of 2-extract five-zone SMB system at the constraint of fixed zone-I flow rate was examined by performing simulation studies for the ternary amino acids (methionine, tryptophan and phenylalanine) system. Product purity values were first evaluated at same safety factor (β) value for all the five zones, then in the second section, the separation performance (purity and recovery values) of the SMB system was investigated under the influence of change in the separation zone safety factor (β_2, β_3 and β_4) values and finally the solutes wave migration behavior were examined at cyclic steady state.

Under the influence of same safety factor (β) value, enhancement in the purity value of methionine and tryptophan occurs with increase in β value, while the purity value of phenylalanine increases up to a value, after that further increase in β value causes a decrease in its purity value due to the diffusion of tryptophan to extract-II column end as result of increase in switching time.

Investigating the effect of change in separation zone safety factor (β_2, β_3 and β_4) values on the separation among methionine, tryptophan and phenylalanine, it was observed that only increase in β_2 value had no effect on purity value of methionine, while the purity value of tryptophan increases and that of phenylalanine decreases. Different purity trends were observed by only changing the β_3 value, purity values of methionine and tryptophan remains almost unchanged while that of phenylalanine increases due to faster migration of solute A wave from the zone-II column end. The results obtained from only increase in safety factor β_4 value effect the product purity value in a manner that the purity value of methionine

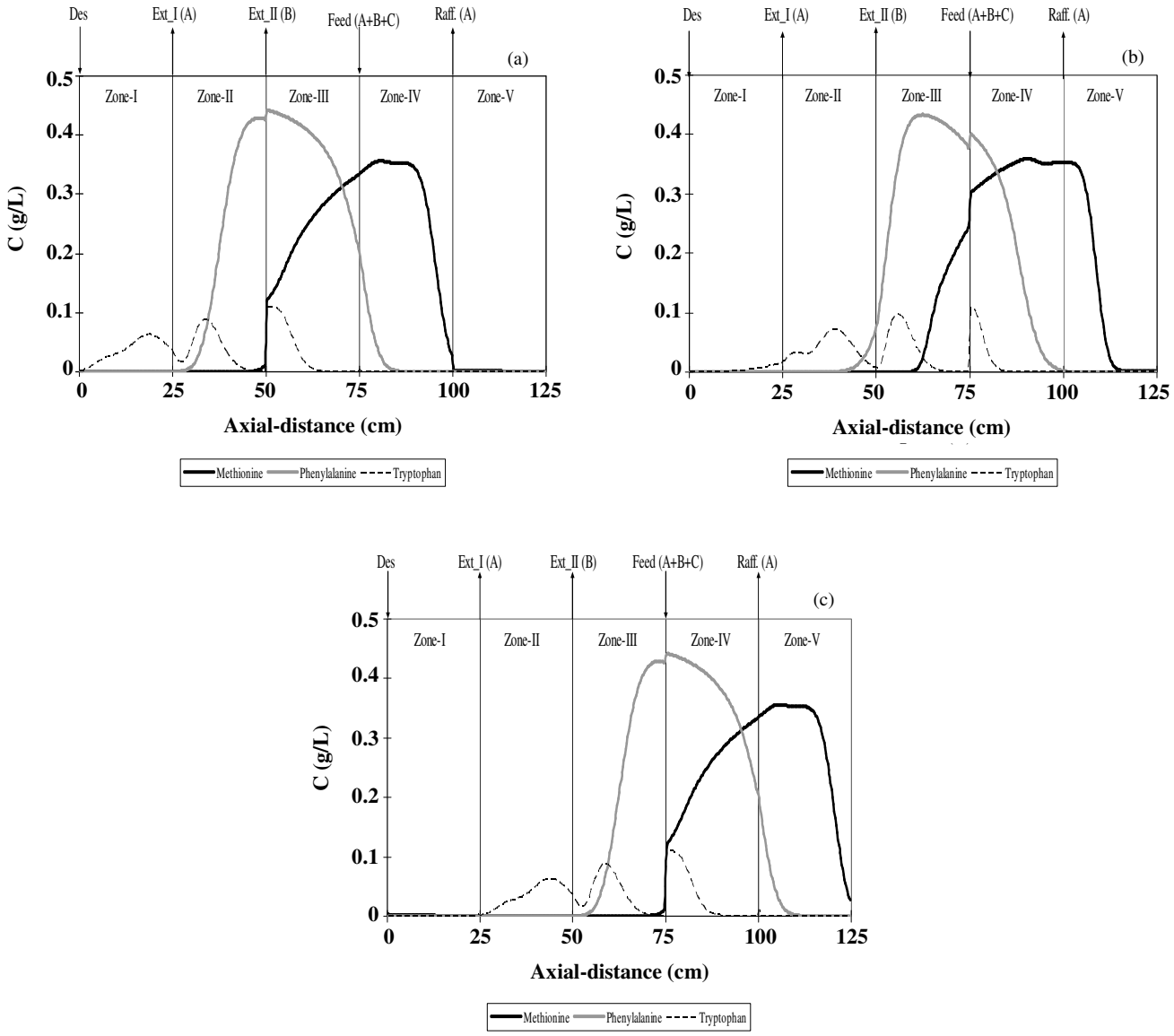

Fig. 7: Solute band migration behavior at cyclic steady state during the entire switching period in a five-zone SMB (a)At the beginning of the period (b) at the middle of the period (c) at the end of the period,. $\beta_3 = 2$, β_1, β_2, β_4, $\beta_5 = 2$, Purity (Methionine =99.74%, Tryptophan = 99.61% and Phenylalanine = 95.47%), P.I value = 98.27%.

increases while that of tryptophan and phenylalanine decreases up to a value, after that the purity values start to increase. Moreover, a general trend of increase in product recovery values was observed with individual increase in separation zone safety factor value. In conclusion it was obvious that the different zone safety facto, β_j (j = 2, 3, 4) value effect the separation performance quite distinctly. However, the results reported are quite promising one in the sense that high product purity and recovery values were obtained for the said amino acid mixture.

The strategy applied in this study (fixed zone-I flow rate) is expected to be highly useful in upgrading the process performance of the current five-zone SMB for separation tasks demanding high purities or high recoveries.

Finally, future research trend for such system can be extended for nonlinear systems. For non linear concentration dependent isotherm systems, a quite different behavior is expected among the components because of competitive effects.

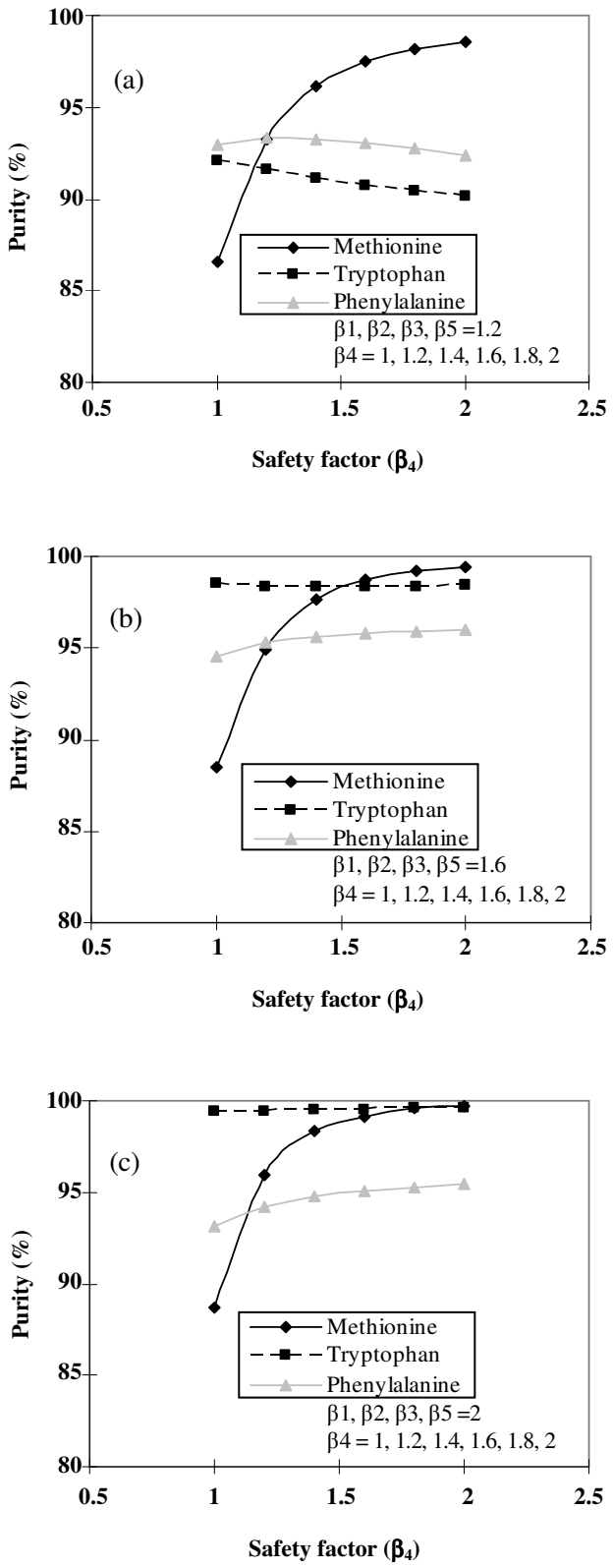

Fig. 8: Influence of change in β_4 value on the separation performance of the 2-extract five-zones SMB.

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Nomenclature

A	Methionine
B	Tryptophan
C	Phenylalanine
a_p	External surface area per particle volume, cm^2/cm^3
C_i	Mobile phase concentration of species i, g/L
d_p	Average particle dia, cm
$E_{b,i}^j$	Axial dispersion coefficient of component i in zone j, cm^2/min
k_m	Mass-transfer coefficient, cm/min
$K_{f,i}$	Lumped mass transfer coefficient, cm^{-1}
K_i	Linear isotherm parameter
P	$(1-\varepsilon) / \varepsilon$ = Phase ratio
PI	Purity index value, %
L_C	Single column length, cm
m_j	Ratio of liquid flow rate to solid phase flow rate in zone j
Q_j^{SMB}	Internal flow rate in each zone, SMB
R	Particle radius, cm
R_{ep}	Reynolds Number
t	Switching time, min
u_i^j	Migration velocity of component i in zone j, cm/min
u_o^j	Mobile phase interstitial velocity in zone j, cm/min
V	Volume of the column, cm^3
v	Port movement velocity, cm/min
Z	Axial position, cm

Greek Letters

β	Safety factor
ε_p	Intra-particle void
ε	Total void fraction

Table 5: Effect of change in β_4 value on the separation performance (recovery) of the 2-extract five-zone SMB.

	Product recovery (%)		
	Raffinate Methionine	Ext_1 Tryptophan	Ext_2 Phenylalanine
$\beta_1, \beta_2, \beta_3, \beta_5 = 1.2$	94.39	94.14	82.21
	93.49	94.84	89.53
	92.62	95.34	92.23
	91.55	95.78	92.99
	90.91	96.01	93.63
	90.05	96.25	93.85
$\beta_1, \beta_2, \beta_3, \beta_5 = 1.6$	98.06	95.18	87.48
	97.91	95.74	94.87
	97.80	96.13	97.59
	97.72	96.41	98.61
	97.66	96.62	99.04
	97.62	96.78	99.34
$\beta_1, \beta_2, \beta_3, \beta_5 = 2$	99.31	93.45	87.28
	99.32	94.59	98.26
	99.31	94.14	98.69
	99.34	94.92	99.05
	99.38	95.16	99.45
	99.72	99.61	99.58

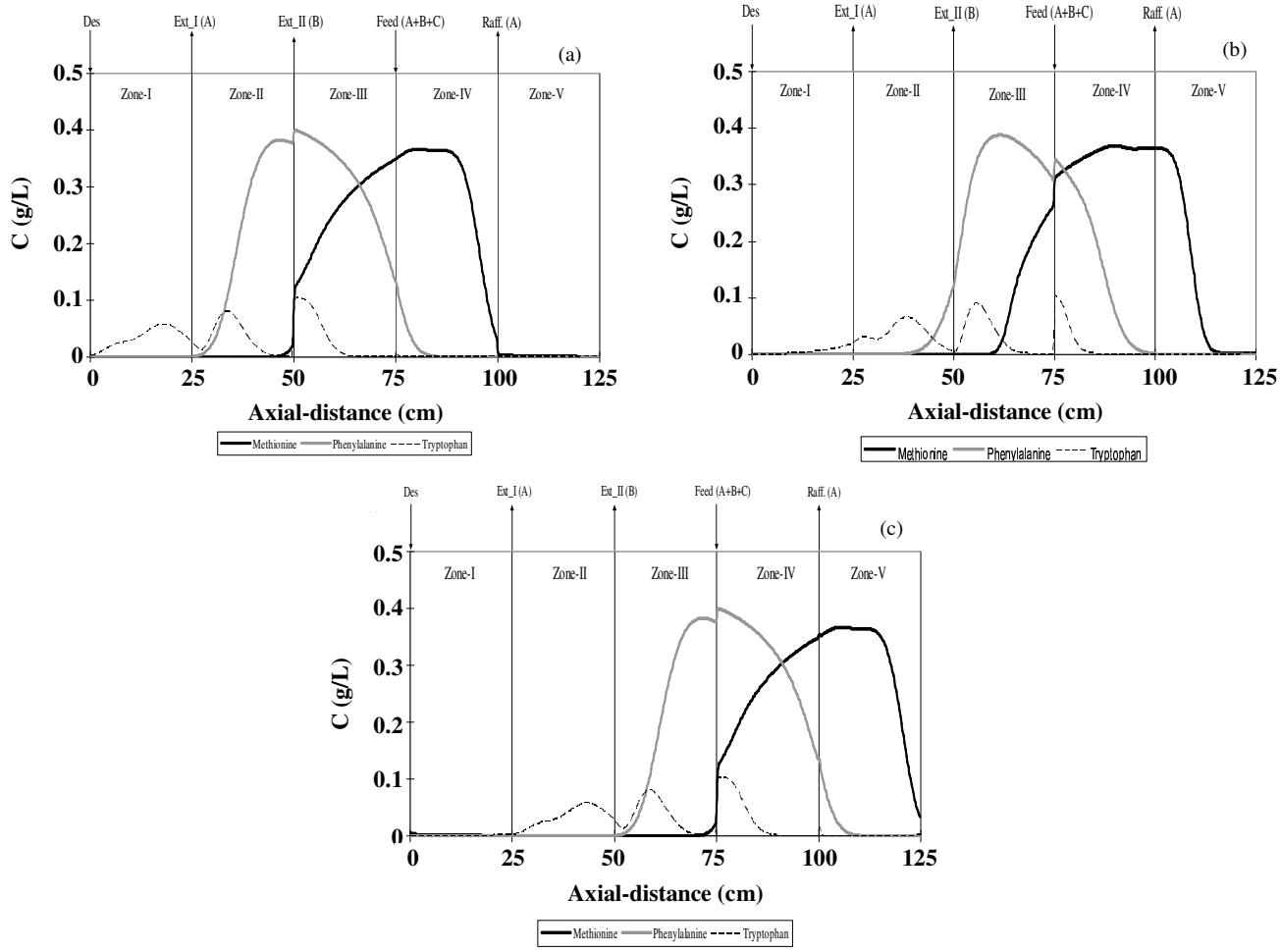

Fig. 9: Solute band migration behavior at cyclic steady state during the entire switching period in a five-zone SMB (a)at the beginning of the period (b) at the middle of the period (c) at the end of the period,. $\beta_4 = 2$, $\beta_1, \beta_2, \beta_3, \beta_5 = 2$, Purity (Methionine =99.64%, Tryptophan = 99.27% and Phenylalanine = 96.03%), P.I value = 98.31%.

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